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FT-IR MEASUREMENTS OF ALIPHATIC AND AROMATIC
C-H GROUPS IN COAL

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ABSTRACT

The experimental difficulties involved in the study of coal structure are both notorious and well-documented. Nevertheless, recent improvements in spectroscopic instrumentation have allowed the determination of what are thought to be reasonably accurate parameters describing an average coal structure. For example, Fourier transform infrared spectroscopy (FT-IR) has been applied to the determination of aromatic and aliphatic hydrogen. Unlike measurements of aromaticity by NMR, however, infrared methods rely on calibrating the intensities of specific bands to the concentration of the appropriate functional groups, using model compounds or other procedures. We have recently found that the values obtained depend heavily on the choice of bands and the methodology employed. In addition, the calibration coefficients vary considerably with rank. We will discuss the various approaches we have employed and the errors involved in each. Our results indicate that the best that can be achieved is the definition of a band of values of aromatic and aliphatic hydrogen.